Available online at www.sciencedirect.com

ScienceDirect

Procedia Engineering 68 (2013) 579 – 585

Procedia Engineering

www.elsevier.com/locate/procedia

The Malaysian International Tribology Conference 2013, MITC2013

A Numerical Model for Wet-Adhesive Line Contact

W.W.F. Chong [a,b,*]

[a] Faculty of Engineering and the Environment, University of Southampton Malaysia Campus (USMC), Nusajaya, Johor, Malaysia
[b] National Centre of Advanced Tribology (nCATS), Faculty of Engineering and the Environment, University of Southampton, Southampton, UK

Abstract

Typical rough surface contact models are meant for dry conditions. They often assume hemispherical shaped asperities when predicting load carrying capacity between the opposing surfaces (e.g. isotropic surfaces). However, modern engineering surfaces are often modified to reduce friction. Surface modifications (e.g. plateau honing in engine cylinder liners) produce anisotropic surfaces, dominated by directional features, resembling ridges. They act as micro-reservoirs, trapping fluids to enhance the lubrication process, leading to lower friction. However, the ridges resemble cylinder-on-a-flat contact, when for example a ring of parabolic face-width profile passes over a cross-hatch honed liner surface. These render the typical rough surface contact models inappropriate when applied to understand the contact behavior of such surfaces. Therefore, as a first approximation to understand anisotropic rough surfaces dominated by directional features, the current study proposes a wet-adhesion line contact model. The model includes the influence of boundary lubrication and asperity adhesion upon the contact load carrying capacity and its deformation. The model considers contribution to boundary lubrication at the assumed smooth summits of asperities due to solvation in diminishing gaps. Solvation has an oscillatory characteristic of fluid molecules. This phenomenon not only generates load carrying capacity, but also prevents direct surface-to-surface interaction. It is also shown that as a result of boundary adsorbed film formation, fluid with long chain molecules and boundary active ends (e.g. 16-mer or hexadecane) has a more significant effect in reducing the chance of adhesion in diminishing gaps, when compared with fluids of simple spherical molecules.

© 2013 The Authors. Published by Elsevier Ltd. Open access under CC BY-NC-ND license.
Selection and peer-review under responsibility of The Malaysian Tribology Society (MYTRIBOS), Department of Mechanical Engineering, Universiti Malaya, 50603 Kuala Lumpur, Malaysia

Keywords: Adhesion; Solvation; Statistical Mechanics; Lennard-Jones; Ornstein-Zernike and Percus-Yevick

Nomenclature

g	Pair correlation function	(-)
$\bar{h}$	Non dimensional deformed profile	(-)
h	Deformed profile	(m)
i, j	Points along simulation domain	(-)
k_B	Boltzmann Constant	($m^2kg.s^{-2}K^{-1}$)

* Corresponding author
E-mail address: w.chong@soton.ac.uk

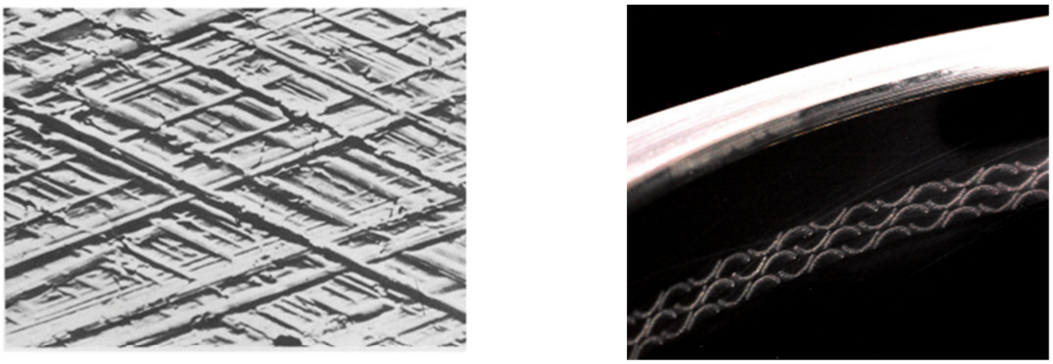
1877-7058 © 2013 The Authors. Published by Elsevier Ltd. Open access under CC BY-NC-ND license.
Selection and peer-review under responsibility of The Malaysian Tribology Society (MYTRIBOS), Department of Mechanical Engineering, Universiti Malaya, 50603 Kuala Lumpur, Malaysia
doi:10.1016/j.proeng.2013.12.224

n	Total number of simulation grid points	(m)
$\overline{p}$	Non dimensional contact pressure	(-)
p	Contact pressure	(Pa)
p_a	Pressure due to adhesion	(Pa)
p_s	Pressure due to solvation	(Pa)
u	Non-deformed contact profile	(m)
$\overline{x}$	Non dimensional simulation domain	(-)
x	Simulation domain	(m)
A	Non dimensional contact state	(-)
C	Influence coefficient	(-)
D	Deformation	(m)
E^*	Reduced modulus Young	(Pa)
F_{err}	Simulation error limit	(-)
F_{res}	Residual function	(-)
R	Contact profile curvature radius	(m)
R_{eff}	Equivalent contact radius	(m)
T	Temperature	(K)
U	Non dimensional undeformed contact profile	(-)
δ	Initial contact state	(m)
ε	Atomic equilibrium spacing	(m)
μ	Tabor's parameter	(-)
ω	Relaxation factor	(-)
$\Delta\gamma$	Surface Energy	(J/m^2)

1. Introduction

Engineering surfaces are microscopically rough, consisting of random features resembling peaks (asperities) and valleys. The geometry of the peaks/asperities is often taken to be hemispherical. Greenwood and Williamson [1] and Greenwood and Tripp [2] proposed rough surface contact models, taking into account asperities to be distributed according to a Gaussian distribution with an average curvature radius. The assumption enables the use of classical Hertzian expressions in predicting load-deflection characteristics of the asperities. However, Nayak [3] showed that the assumption of Gaussian distributed asperities with an average curvature radius is not valid for all engineering surfaces. Besides showing that surface features are multi-scale, Sayles and Thomas [4] also observed similar trends as suggested by Nayak [3]. These observations lead to the developments of better rough surface models such as the use of fractal analysis by Majumdar and Bhushan [5], Yan and Komvopoulos [6] and lately Chong et al [7].

The aforementioned models consider elastoplastic deformation of asperities with hemispherical geometry at varying curvature radii. However, nowadays, intentional surface features are manufactured onto engineering surfaces, creating lubrication micro-reservoirs that reduce friction. The approach is commonly used in engine cylinder liners through plateau honing [8] (figure 1(a)) and laser etching along top dead centers of the liners [9] (figure 1(b)). As a result of directionality/anisotropic roughness introduced onto the engineering surface, hemispherical asperity assumption is no longer applicable in predicting contact characteristics along such surfaces. For example, the surface topography post plateau honing (figure 1(a)) resemble a cylinder-on-a-flat contact rather than a hemispherical asperity. The advancement in friction reduction shows the need to also consider cylinder-on-a-flat (line) contact models for a rough surface analysis.



a. Plateau honing [8] b. Laser etching along top dead center of cylinder liners

Fig. 1. Surface modifications on engine cylinder liner to reduce friction

The gap between a pair of opposing rough surfaces in relative motion is dominated by boundary friction. Besides being rarely smooth, engineering surfaces are also rarely dry. The surface wetness can be intentional (lubrication) or unintentional through condensation. In lubrication, additives such as friction modifiers are usually included in a fully formulated lubricant blend to reduce boundary friction. Friction modifiers, consisting of molecules with boundary active ends adsorb to the surface and act as a last barrier in preventing direct surface-to-surface interaction [10] (figure 2).

Besides surface adsorption, in diminishing gaps of several molecular diameters, the density distribution of additive molecules near the smooth solid surfaces differs from that in the bulk of any thin film formed [11]. This phenomenon gives rise to an attractive-repulsive kinetic interaction known as solvation [12]. The effect of solvation towards the contact characteristics (e.g. deformation) is shown to be significant experimentally by Chan and Horn [13] and Horn and Israelachvilli [14], and by Matsuoka and Kato [15], Al-Samieh and Rahnejat [16-18] and Chong et al [19] through numerical analyses using an empirical relationship for the generated solvation pressure.

Once the contact penetrates the boundary film, boundary adhesion between opposing surfaces will dominate the contact behavior (figure 2). Typical models that consider dry boundary adhesion include JKR [20], DMT [21] and Maugis-Dugdale [22]. The JKR model is best suited to larger-radius compliant solids with more compliant materials such as rubber, whilst the DMT is suitable for stiff materials with smaller radii. As JKR and DMT adhesion models work on both extreme ends of the contact conditions, Maugis' model fills the transitional gap between them. However, the drawback of these models is that load-deflection characteristics, mainly as a result of the attraction between materials of opposing surfaces without any consideration of a boundary adsorbed film as shown in figure 2.

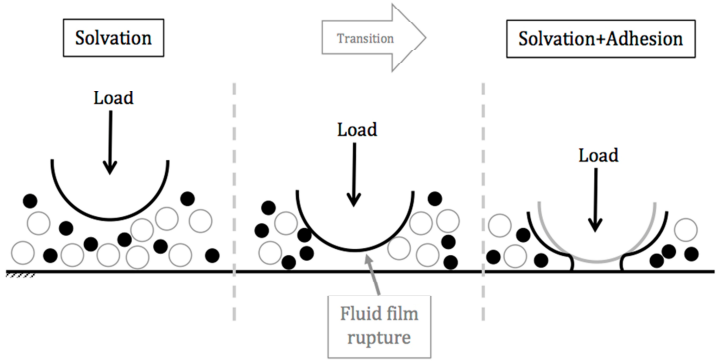


Fig. 2. Contact transition from wet to dry adhesion

Therefore, as a first approximation to model anisotropic rough surface contacts, the current study proposes a wet adhesion line contact model to predict the combined influence of boundary lubrication and adhesion for a cylinder-on-a-flat (line) contact. The proposed model can be extended for application for typical rough surface models as discussed earlier.

2. Mathematical Model

The study attempts to model a cylinder-on-a-flat, resembling a line contact. The cross-section of the cylinder is assumed to be semi-circle having curvature radius, R. The contact profile, $h(x)$ is expressed as

$$h(x) = u(x) + D(x) + \delta \tag{1}$$

With u $(= R - \sqrt{R^2 - x^2})$ being the non-deformed profile, δ refers to the initial contact state of the cylinder-on-a-flat. The term, D is the contact deflection and is described as [23]:

$$D(x)|_{x=idx} = \frac{8\mu^{3/2}}{3\pi}\sum_{j=1}^{n} C_{ij}.p_j; \quad \mu = \left(\frac{R\Delta\gamma^2}{E^{*2}\varepsilon^3}\right)^{1/3} \tag{2}$$

Where C is called the influence coefficient matrix [24] and μ is referred to as the Tabor's parameter. The schematic diagram showing the simulated contact problem is included in figure 3.

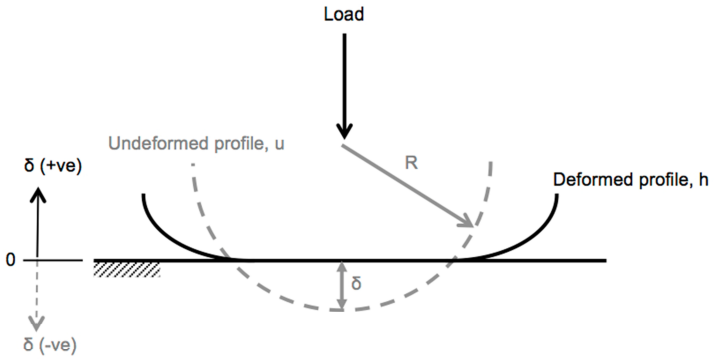


Fig. 3. Schematic diagram of simulated contact

The total contact pressure, *p(x)* consists of two terms, namely the solvation pressure, p_s and adhesion pressure, p_a .

$$p(x) = p_a(x) + p_s(x) \tag{3}$$

In this study, the solvation pressure is computed using the method proposed by Chong et al [25, 26]. The model is also capable of predicting boundary adsorbed film formation for linear chain molecules. The statistical mechanics-based solution is based on the Ornstein-Zernike equation [27] coupled with the Percus-Yevick [28] approximation to obtain the pair correlation function, *g*. The pair correlation function, *g* describes the possibility of finding a molecule, A from a reference molecule, B in a given volume. Using the approximated pair correlation function, the solvation pressure is defined as:

$$p_s(\mathrm{x}) = -\frac{d^2}{dx^2}\frac{1}{2\pi R_{eff}}[k_B T(g(\mathrm{x}) - 1)] \tag{4}$$

The adhesive component of the contact pressure is computed using the Lennard-Jones potential rather than the classical JKR, DMT or the Maugis-Dugdale approach. The contact pressure due to boundary adhesion is as follow [23]:

$$p_a(x) = \frac{8\Delta\gamma}{3\varepsilon}\left\{\left[\frac{\varepsilon}{h(x)}\right]^3 - \left[\frac{\varepsilon}{h(x)}\right]^9\right\} \tag{5}$$

Where $\Delta\gamma$ is the surface energy and ε refers to the atomic equilibrium spacing.

2.1. Numerical Procedure

The line contact model in this study applies the discretization as follow [23]:

$$\overline{x} = \frac{x}{\sqrt{\varepsilon R}};\quad U = \frac{u}{\varepsilon};\quad A = \frac{\delta}{\varepsilon};\quad \overline{p} = \left(\frac{\varepsilon}{\Delta\gamma}\right)p;\quad \overline{h} = \frac{h}{\varepsilon} - 1$$

To obtain the total pressure and deformed profile of the simulated contact, the approach proposed by Feng [23] is applied. The numerical approach based on Newton's method of iteration gives the residual term, F_{res} as:

$$F_{res} = \overline{h}(\overline{x}) + D(\overline{x}) - U(\overline{x}) + A \approx 0 \tag{6}$$

The numerical procedure for the simulated contact is summarized as follow in figure 4.

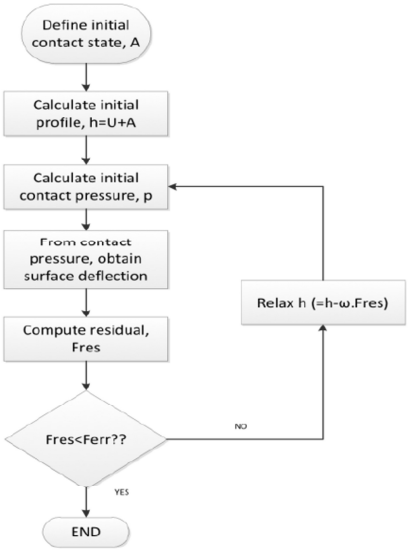


Fig. 4. Flow chart for numerical solution

3. Results and Discussions

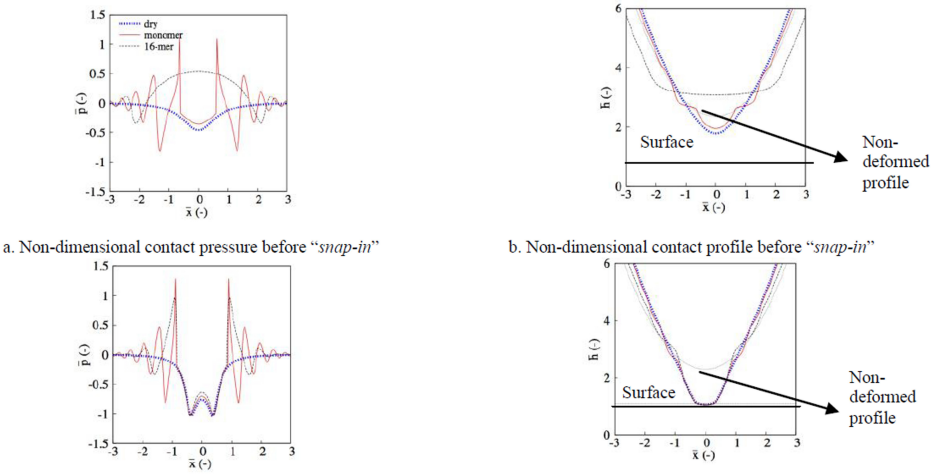
For the simulated line contact, the parameters used are: curvature radius, R= *20*nm, atomic equivalent spacing, ε=*0.235* nm, relaxation factor, $\omega = 1.0\times10^{-3}$ and $F_{err} = 1.0\times10^{-6}$ for 500 grid points. Figure 5(a) shows the change in load per unit length in the function of the contact's given initial state, δ for a dry contact. With an increase in surface energy, Δγ, the role of adhesive force is enhanced, leading to a "*snap-in*" to the contact scenario, which is often used to understand the "*pull-off*" force of an adhering contact. However, once a fluid is introduced to the contact, the influence of near-surface adhesion for the same contact geometry reduces (figure 5(b)). This is observed that by introducing a fluid with linear chain molecules having boundary active ends (*16-mer*, e.g. hexadecane), the contact becomes less "*sticky*" as compared with a fluid with simple spherical molecules (*monomer*). This is because of the adsorbed boundary film formed from the fluid with linear chain molecules, which prevents direct surface-to-surface interaction, leading to lower friction. This observation is in accord with the selection criteria for friction modifiers in fully formulated lubricant blends, where boundary active and linear short chain molecules have been observed to reduce friction more effectively as compared with complex molecules (e.g. long chain and branched molecules) [26,29,30].

a. Surface energy variation

b . Fluid molecular chain-length variation

Fig. 5. Contact load variation with initial contact state, δ

The pressure distribution and deformed profile of the contact, when "*snap-in*" occurs are shown in figure 5. Before "*snap-in*" (figure 6(a) and (b)), it is shown that the contacting surfaces are separated by the fluid with *16-mer* molecules and undergoes less oscillatory pressure, but with a larger contact deflection. This is because long chain molecules inhibit oscillations (as a result of molecular restructuring within the contact). In figure 6(c) and (d) when "*snap-in*" occurs, it is observed that the contact for dry and wet conditions is being pulled to the surface. However, the fluid molecules surrounding the non-contact area still provide load carrying capacity, evidently shown through the profile deformations in a stepwise manner due to the solvation effect (figure 6(d)).



a. Non-dimensional contact pressure before "*snap-in*"

b. Non-dimensional contact profile before "*snap-in*"

c. Non-dimensional contact pressure after "*snap-in*"

d. Non-dimensional contact profile after "*snap-in*"

Fig. 6. Pressure and profile before and after "*snap-in*" of the contact

4. Conclusion

The study shows the influence of both boundary lubrication (induced by solvation and adsoprtion) and boundary adhesion upon the contact pressure and profile deformation of a line contact. It is observed that introducing a fluid within the contact of a pair of opposing surfaces affects the "*stickiness*" of the contact. Fluids with long chain molecules, having boundary active molecular ends demonstrate significant influence on the adhesion and deflection of the contact when compared with those with simple spherical molecules.

Acknowledgments

The author acknowledges the support provided by the Malaysian Ministry of Education under the Fundamental Research Grant Scheme (FRGS) through the *n-SIMPAC* project and the Exploratory Research Grant Scheme (ERGS) through *The Design of Lubricant and Surface Interaction for Reduced Boundary Friction and Wear* project.

References

[1] Greenwood J.A. and Williamson B.P. *Contact between nominally flat surfaces*. Proc. Roy. Soc. Ser. A, 24:300–319,1966.
[2] Greenwood J. A. and Tripp J. H. *The contact of two nominally flat rough surfaces*. Proc. IMechE, 185:625–633, 1970.
[3] Nayak P. R. *Random pressure model of rough surfaces*. Trans ASME, J. Lubn. Tech., 93(3):398–407, 1971.
[4] Sayles R. S. and Thomas T. R. *Surface topography as a non-stationary random process*. Nature, 271:431–434, 1971.
[5] Majumdar A. and Bhushan B. *Fractal model of elastic-plastic contact between rough surfaces*. Trans ASME, J. Trib., 113(1):1–11, 1991.
[6] Yan W. and Komvopoulos K. *Contact analysis of elastic-plastic fractal surfaces*. J. Phys., D: Appl. Phys., 84(7):3617 3624, 1998.
[7] Chong W. W. F., Teodorescu M., and Rahnejat H. *Nanoscale elastoplastic adhesion of wet asperities*. Proc. IMechE. Part J: Journal of Engineering Tribology, 2013 (doi: 10.1177/1350650112472142)
[8] Willis E. *Surface finish in relation to cylinder liners*. Wear, 109:351–366, 1986.
[9] Rahnejat H., Balakrishnan S., King P. D., and Howell-Smith S. *In-cylinder friction reduction using a surface finish optimization technique*. Proc IMechE, Part D: J. Automobile Eng, 220(9):1309–1318, 2006.
[10] Hardy W. B. and Doubleday I. *Boundary lubrication - the paraffin series*. Proc. Roy. Soc. London, Series A, 100:550–574, 1921.
[11] Israelachvili J. N. *Intermolecular and surface forces*. Academic press, New York, 1992.
[12] Gohar R. and Rahnejat H. Fundamentals of Tribology. Imperial College Press, London, 2008.
[13] Chan D.Y.C. and Horn R.G. *The drainage of thin liquid films between solid surfaces*. J.Chem.Phys., 83(10):5311–5324, 1985.
[14] Horn R. G. and Israelachvili J. N. *Direct measurement of structural forces between two surfaces in a nonpolar liquid*. J. Chem. Phys., 75(3):1400–1412, 1981.
[15] Matsuoka H. and Kato T. *An ultrathin liquid film lubrication theory - calculation method of solvation pressure and its application to the ehl problem*. Trans ASME, J. Trib., 119:217–226, 1997.
[16] Al-Samieh M. and Rahnejat H. *Ultra-thin lubricating films under transient conditions*. J. Phys., D: Appl. Phys., 34:2610–2621, 2001.
[17] Abd. Al-Samieh M. F. and Rahnejat H. *Nano-lubricant film formation due to combined elastohydrodynamics and surface force action under isothermal conditions*. Proc. IMechE, Part C : J. Mech. Eng. Sci., 215:1019–1029, 2001.
[18] Al-Samieh M. and Rahnejat H. *Physics of lubricated impact of a sphere in a plate in a narrow continuum to gaps of molecular dimensions*. J. Phys., D: Appl. Phys., 35:2311–2326, 2002.
[19] Chong W. W. F., Teodorescu M., and Rahnejat H. *Effect of lubricant molecular rheology on formation and shear of ultra-thin surface films*. J. Phys., D: Appl. Phys., 44(16):165302, 2011.
[20] Johnson K. L., Kendall K., and Roberts A. D. *Resolving the contradiction of asperities plastic to elastic mode transition in current contact models of fractal rough surfaces*. Proc. Roy. Soc., Series A, pages 301–313, 1971.
[21] Derjaguin B. V., Muller V. M., and Toporov Y. P. *Effect of contact deformation on the adhesion of elastic solids*. J. Colloid and Interface Sci., 53:314–326, 1975.
[22] Maugis D. On the contact and adhesion of rough surfaces. J. Adhesion Sci. & Tech., 10(2):161–175, 1996.
[23] Feng J. Q. *Contact behavior of spherical elastic particles: a computational study of particle adhesion and deformations.* Colloids and Surface A: Physicochem. and Eng. Asp., 172:175-198, 2000.
[24] L. G. Houpert and B. J. Hamrock. *Fast approach for calculating film thicknesses and pressures in elastohydrodynamically lubricated contacts at high loads*. Journal of Tribology, 108(3):411–419, 1986.
[25] Chong W. W. F., Teodorescu M., and Rahnejat H. *Formation of ultra-thin bi-molecular boundary adsorbed films*. J. Phys., D: Appl. Phys., 45(11):115303, 2012.
[26] Chong W. W. F.,Teodorescu M. and Rahnejat H. *Physio-chemical hydrodynamic mechanism underlying the formation of thin adsorbed boundary films*. Roy. Soc. Chem. : Faraday Discussion 156 Tribology, 2011.
[27] Ornstein L. S. and Zernike F. *Accidental deviations of density and opalescence at the critical point of a single substance*. Proc. Roy. Acad., Amsterdam, 17:793–806, 1914.
[28] Percus K. and Yevick G. J., *Analysis of classical statistical mechanics by means of collective coordinates*. Phy. Rev,110:1–13, 1958.
[29] Wu, Y. L., and Dacre, B., 1997. "Effects of lubricant- additives on the kinetics and mechanisms of zddp ad- sorption on steel surfaces". *Tribology International, 30*, pp. 445–453.
[30] Tung, S. C., and Gao, H., 2002. "Tribological investigation of piston ring coatings operating in an alternative fuel and engine oil blend". *Tribology Trans, 45*(3), pp. 381–9.